

## Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTADEG1625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* \* \* \* \* \* \* \* \* \* \* STN Columbus \* \* \* \* \* \* \* \* \* \* \* \* \*

FILE 'HOME' ENTERED AT 15:09:42 ON 26 MAR 2007

=> file registry	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:09:58 ON 26 MAR 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 25 MAR 2007 HIGHEST RN 928121-90-8  
DICTIONARY FILE UPDATES: 25 MAR 2007 HIGHEST RN 928121-90-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

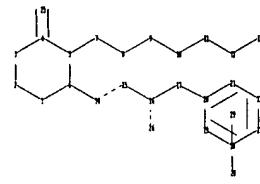
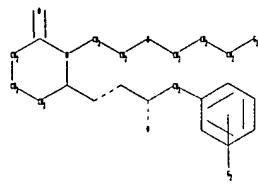
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10-564829 gen.str



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 25 26 28

ring nodes :

1 2 3 4 5 6 18 19 20 21 22 23

chain bonds :

4-25 5-7 6-14 7-8 8-9 9-10 10-11 11-12 12-13 14-15 15-16 16-17 16-26

17-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 4-25 5-6 12-13 14-15 16-26

exact bonds :

5-7 6-14 7-8 8-9 9-10 10-11 11-12 15-16 16-17 17-20

normalized bonds :

18-19 18-23 19-20 20-21 21-22 22-23

G1:C,S,P

G2:C,O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom  
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 25:CLASS 26:CLASS 28:CLASS 29:Atom

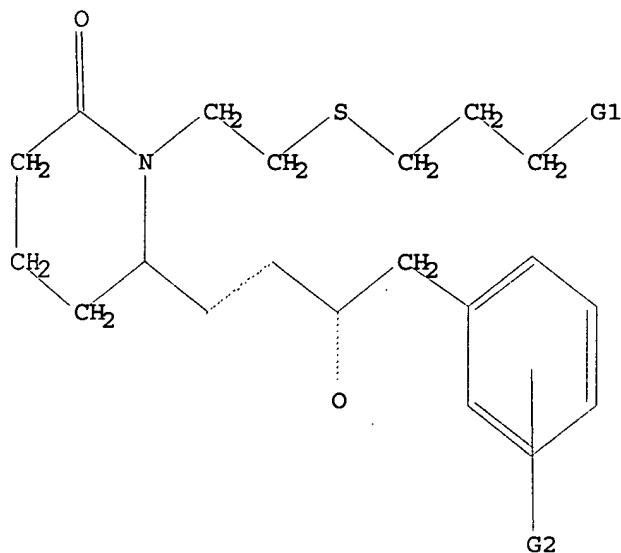
L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1

STR



G1 C,S,P

G2 C,O,N

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 15:11:08 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 26 TO ITERATE

100.0% PROCESSED 26 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 215 TO 825  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> d scan  
L2 HAS NO ANSWERS

=> s 11 sss full  
FULL SEARCH INITIATED 15:11:46 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 327 TO ITERATE

100.0% PROCESSED 327 ITERATIONS  
SEARCH TIME: 00.00.02

1 ANSWERS

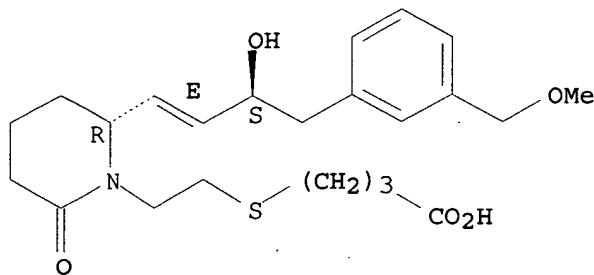
L3 1 SEA SSS FUL L1

=> d scan

L3 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-3-hydroxy-4-[3-(methoxymethyl)phenyl]-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI)  
MF C23 H33 N O5 S

Absolute stereochemistry.

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> d 13 full ibib hitstr  
'FULL' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'  
'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'  
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG	- RN
SAM	- Index Name, MF, and structure - no RN
FIDE	- All substance data, except sequence data
IDE	- FIDE, but only 50 names
SQIDE	- IDE, plus sequence data
SQIDE3	- Same as SQIDE, but 3-letter amino acid codes are used
SQD	- Protein sequence data, includes RN
SQD3	- Same as SQD, but 3-letter amino acid codes are used
SQN	- Protein sequence name information, includes RN
CALC	- Table of calculated properties
EPROP	- Table of experimental properties
PROP	- EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS	-- Abstract
APPS	-- Application and Priority Information
BIB	-- CA Accession Number, plus Bibliographic Data
CAN	-- CA Accession Number
CBIB	-- CA Accession Number, plus Bibliographic Data (compressed)
IND	-- Index Data
IPC	-- International Patent Classification
PATS	-- PI, SO
STD	-- BIB, IPC, and NCL
IABS	-- ABS, indented, with text labels
IBIB	-- BIB, indented, with text labels
ISTD	-- STD format, indented
OBIB	----- AN, plus Bibliographic Data (original)

OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.

HELP FORMATS -- To see detailed descriptions of the predefined formats.

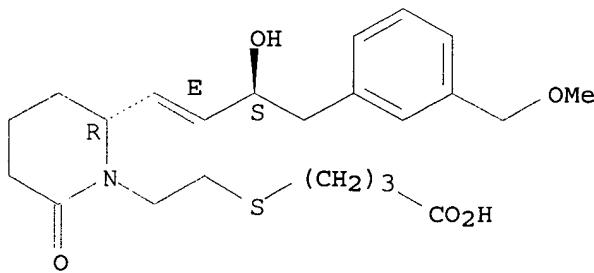
ENTER DISPLAY FORMAT (IDE):end

=> d 13 1 IDE

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 724705-74-2 REGISTRY  
ED Entered STN: 10 Aug 2004  
CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-3-hydroxy-4-[3-(methoxymethyl)phenyl]-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]-(9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C23 H33 N O5 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
179.00	179.21

FILE 'CAPLUS' ENTERED AT 15:17:18 ON 26 MAR 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is

held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 26 Mar 2007 VOL 146 ISS 14  
FILE LAST UPDATED: 25 Mar 2007 (20070325/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> d history

(FILE 'HOME' ENTERED AT 15:09:42 ON 26 MAR 2007)

FILE 'REGISTRY' ENTERED AT 15:09:58 ON 26 MAR 2007

L1                   STRUCTURE UPLOADED  
L2                   0 S L1 SSS SAM  
L3                   1 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 15:17:18 ON 26 MAR 2007

=> s l3  
L4                   2 L3

=> d l3 all ibib abs hitstr

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:Y

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG	- RN
SAM	- Index Name, MF, and structure - no RN
FIDE	- All substance data, except sequence data
IDE	- FIDE, but only 50 names
SQIDE	- IDE, plus sequence data
SQIDE3	- Same as SQIDE, but 3-letter amino acid codes are used
SQD	- Protein sequence data, includes RN
SQD3	- Same as SQD, but 3-letter amino acid codes are used
SQN	- Protein sequence name information, includes RN
CALC	- Table of calculated properties
EPROP	- Table of experimental properties
PROP	- EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS	-- Abstract
APPS	-- Application and Priority Information
BIB	-- CA Accession Number, plus Bibliographic Data
CAN	-- CA Accession Number

CBIB -- CA Accession Number, plus Bibliographic Data (compressed)  
IND -- Index Data  
IPC -- International Patent Classification  
PATTS -- PI, SO  
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels  
IBIB -- BIB, indented, with text labels .  
ISTD -- STD format, indented  
  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.  
HELP FORMATS -- To see detailed descriptions of the predefined formats.  
ENTER DISPLAY FORMAT (IDE):end

FILE 'CAPLUS' ENTERED AT 15:19:35 ON 26 MAR 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 26 Mar 2007 VOL 146 ISS 14  
FILE LAST UPDATED: 25 Mar 2007 (20070325/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> d history

(FILE 'HOME' ENTERED AT 15:09:42 ON 26 MAR 2007)

FILE 'REGISTRY' ENTERED AT 15:09:58 ON 26 MAR 2007

L1 STRUCTURE uploaded  
L2 0 S L1 SSS SAM

L3 1 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 15:17:18 ON 26 MAR 2007

L4 2 S L3

FILE 'REGISTRY' ENTERED AT 15:19:21 ON 26 MAR 2007

FILE 'CAPLUS' ENTERED AT 15:19:26 ON 26 MAR 2007

FILE 'CAPLUS' ENTERED AT 15:19:35 ON 26 MAR 2007

=> d l3 1-2 ibib abs hitst

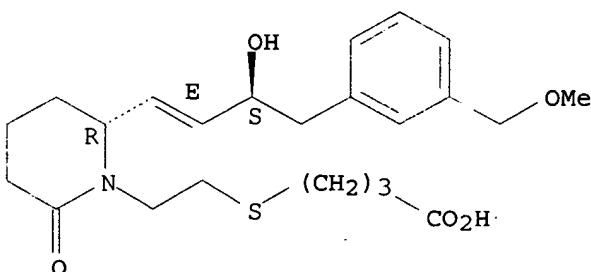
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

=> d l4 1-2 ibib hitstr

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2005:378879 CAPLUS  
DOCUMENT NUMBER: 143:59790  
TITLE: Lactams as prostanoid receptor ligands. Part 4:  
2-Piperidones as selective EP4 receptor agonists  
AUTHOR(S): Elworthy, Todd R.; Brill, Emma R.; Caires, Christopher  
C.; Kim, Woongki; Lach, Leang K.; Tracy, Jahari  
Laurant; Chiou, San-San  
CORPORATE SOURCE: Roche Palo Alto, Department of Medicinal Chemistry,  
Palo Alto, CA, 94304-1397, USA  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),  
15(10), 2523-2526  
CODEN: BMCL8; ISSN: 0960-894X  
PUBLISHER: Elsevier B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 143:59790  
IT 724705-74-2P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL  
(Biological study); PREP (Preparation)  
(stereoselective preparation and EP4 receptor binding affinity of  
piperidones starting from amino adipic acid using resolution as the key  
step)  
RN 724705-74-2 CAPLUS  
CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-3-hydroxy-4-[3-  
(methoxymethyl)phenyl]-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2004:589253 CAPLUS

DOCUMENT NUMBER: 141:123513  
 TITLE: 2-piperidone derivatives as prostaglandin agonists  
 INVENTOR(S): Elworthy, Todd Richard  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 26 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004142969	A1	20040722	US 2004-754117	20040108
AU 2004203905	A1	20040729	AU 2004-203905	20040102
CA 2511255	A1	20040729	CA 2004-2511255	20040102
WO 2004063158	A1	20040729	WO 2004-EP8	20040102
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ			
EP 1585729	A1	20051019	EP 2004-700041	20040102
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2004006717	A	20051220	BR 2004-6717	20040102
CN 1735597	A	20060215	CN 2004-80002071	20040102
JP 2006515015	T	20060518	JP 2005-518636	20040102
PRIORITY APPLN. INFO.:			US 2003-439152P	P 20030110
			WO 2004-EP8	W 20040102

OTHER SOURCE(S): MARPAT 141:123513

IT 724705-74-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

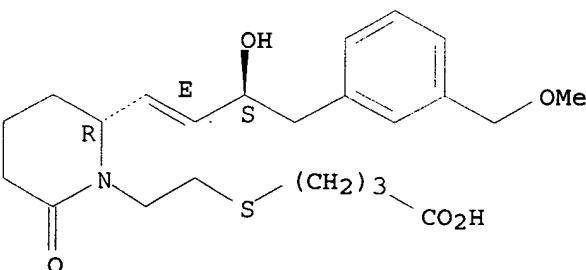
(preparation of 2-piperidone derivs. as selective prostaglandin EP4 agonists for the treatment of associated diseases)

RN 724705-74-2 CAPLUS

CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-3-hydroxy-4-[3-(methoxymethyl)phenyl]-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



=> logoff hold

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
13.35	194.89

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 15:27:11 ON 26 MAR 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAEG1625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* \* \* \* \* Welcome to STN International \* \* \* \* \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 DEC 18 CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role  
NEWS 4 DEC 18 CA/CAplus patent kind codes updated  
NEWS 5 DEC 18 MARPAT to CA/CAplus accession number crossover limit increased to 50,000  
NEWS 6 DEC 18 MEDLINE updated in preparation for 2007 reload  
NEWS 7 DEC 27 CA/CAplus enhanced with more pre-1907 records  
NEWS 8 JAN 08 CHEMLIST enhanced with New Zealand Inventory of Chemicals  
NEWS 9 JAN 16 CA/CAplus Company Name Thesaurus enhanced and reloaded  
NEWS 10 JAN 16 IPC version 2007.01 thesaurus available on STN  
NEWS 11 JAN 16 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data  
NEWS 12 JAN 22 CA/CAplus updated with revised CAS roles  
NEWS 13 JAN 22 CA/CAplus enhanced with patent applications from India  
NEWS 14 JAN 29 PHAR reloaded with new search and display fields  
NEWS 15 JAN 29 CAS Registry Number crossover limit increased to 300,000 in multiple databases  
NEWS 16 FEB 15 PATDPASPC enhanced with Drug Approval numbers  
NEWS 17 FEB 15 RUSSIAPAT enhanced with pre-1994 records  
NEWS 18 FEB 23 KOREAPAT enhanced with IPC 8 features and functionality  
NEWS 19 FEB 26 MEDLINE reloaded with enhancements  
NEWS 20 FEB 26 EMBASE enhanced with Clinical Trial Number field  
NEWS 21 FEB 26 TOXCENTER enhanced with reloaded MEDLINE  
NEWS 22 FEB 26 IFICDB/IFIPAT/IFIUDB reloaded with enhancements  
NEWS 23 FEB 26 CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases  
NEWS 24 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format  
NEWS 25 MAR 16 CASREACT coverage extended  
NEWS 26 MAR 20 MARPAT now updated daily  
NEWS 27 MAR 22 LWPI reloaded  
  
NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8  
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* \* \* \* \* \* \* \* \* \* \* STN Columbus \* \* \* \* \* \* \* \* \* \* \* \* \*

FILE 'HOME' ENTERED AT 15:22:38 ON 27 MAR 2007

=> registry

REGISTRY IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.  
For a list of commands available to you in the current file, enter  
"HELP COMMANDS" at an arrow prompt (=>).

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n) :

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:23:17 ON 27 MAR 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 MAR 2007 HIGHEST RN 928196-39-8

DICTIONARY FILE UPDATES: 26 MAR 2007 HIGHEST RN 928196-39-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

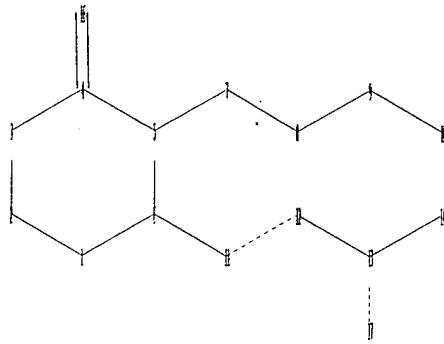
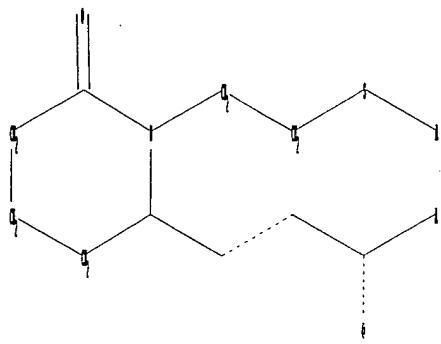
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10-564829 genA.str



chain nodes :

7 8 9 10 11 12 13 14 16 17

ring nodes :

1 2 3 4 5 6

chain bonds :

4-16 5-7 6-11 7-8 8-9 9-10 11-12 12-13 13-14 13-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 4-16 5-6 9-10 11-12 13-14 13-17

exact bonds :

5-7 6-11 7-8 8-9 12-13

G1:C,S,P

G2:C,O,N

Match level :

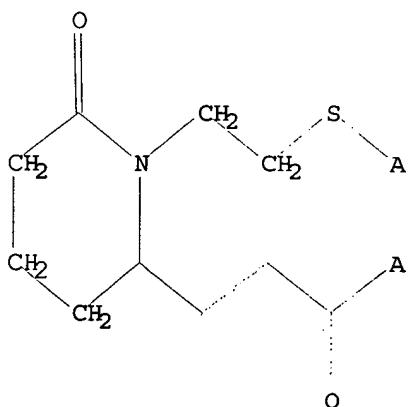
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 16:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 C,S,P

G2 C,O,N

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 15:24:12 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 49 TO ITERATE

100.0% PROCESSED 49 ITERATIONS  
SEARCH TIME: 00.00.01

2 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 560 TO 1400  
PROJECTED ANSWERS: 2 TO 124

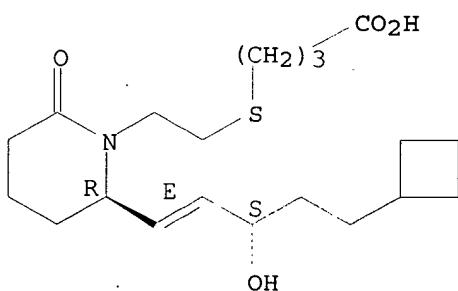
L2 2 SEA SSS SAM L1

=> d scan

L2 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-5-cyclobutyl-3-hydroxy-1-pentenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI)  
MF C20 H33 N O4 S

Absolute stereochemistry.

Double bond geometry as shown.



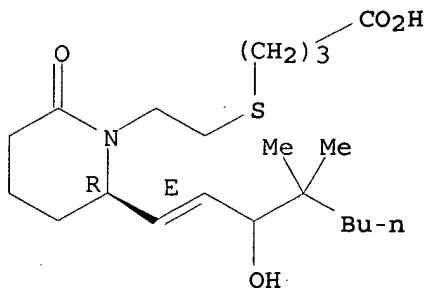
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Butanoic acid, 4-[[2-[(2R)-2-[(1E)-3-hydroxy-4,4-dimethyl-1-octenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI)  
MF C21 H37 N O4 S

Absolute stereochemistry.

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s 11 sss full  
 FULL SEARCH INITIATED 15:25:19 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 771 TO ITERATE

100.0% PROCESSED 771 ITERATIONS  
 SEARCH TIME: 00.00.01

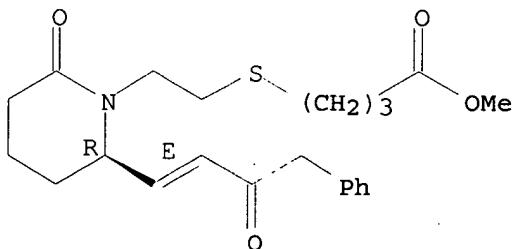
12 ANSWERS

L3 , 12 SEA SSS FUL L1

=> d 13

L3 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 871578-35-7 REGISTRY  
 ED Entered STN: 10 Jan 2006  
 CN Butanoic acid, 4-[[2-[(6R)-2-oxo-6-[(1E)-3-oxo-4-phenyl-1-butenyl]-1-piperidinyl]ethyl]thio]-, methyl ester (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C22 H29 N O4 S  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

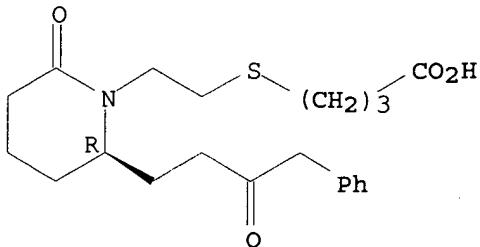
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d 13 2-12

L3 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN

RN 871578-30-2 REGISTRY  
 ED Entered STN: 10 Jan 2006  
 CN Butanoic acid, 4-[[2-[(6R)-2-oxo-6-(3-oxo-4-phenylbutyl)-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C21 H29 N O4 S  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

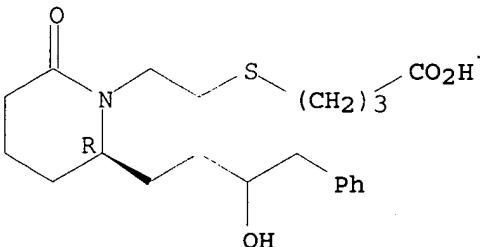


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 871578-29-9 REGISTRY  
 ED Entered STN: 10 Jan 2006  
 CN Butanoic acid, 4-[[2-[(2R)-2-(3-hydroxy-4-phenylbutyl)-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C21 H31 N O4 S  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



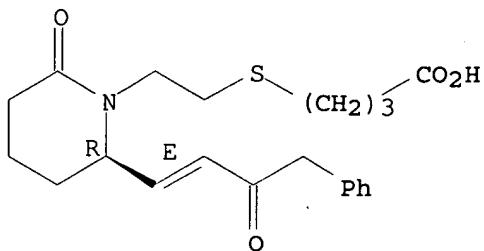
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 871578-28-8 REGISTRY  
 ED Entered STN: 10 Jan 2006  
 CN Butanoic acid, 4-[[2-[(6R)-2-oxo-6-[(1E)-3-oxo-4-phenyl-1-butenyl]-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C21 H27 N O4 S  
 SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.  
Double bond geometry as shown.

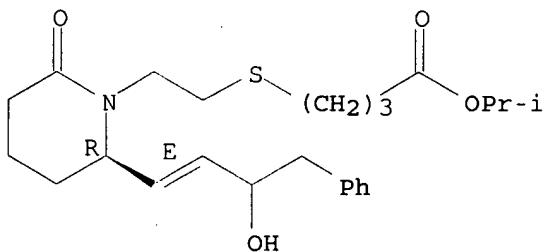


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 871578-27-7 REGISTRY  
ED Entered STN: 10 Jan 2006  
CN Butanoic acid, 4-[[2-[(2R)-2-[(1E)-3-hydroxy-4-phenyl-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]-, 1-methylethyl ester (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H35 N O4 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.  
Double bond geometry as shown.

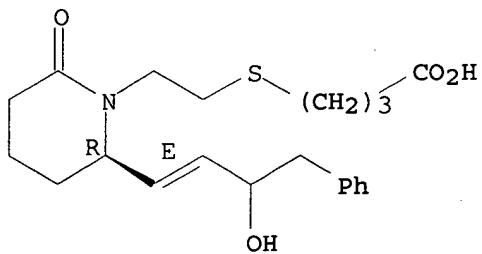


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 871578-26-6 REGISTRY  
ED Entered STN: 10 Jan 2006  
CN Butanoic acid, 4-[[2-[(2R)-2-[(1E)-3-hydroxy-4-phenyl-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C21 H29 N O4 S  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.  
Double bond geometry as shown.

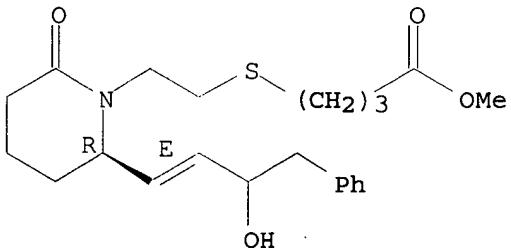


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 871578-25-5 REGISTRY  
 ED Entered STN: 10 Jan 2006  
 CN Butanoic acid, 4-[[2-[(2R)-2-[(1E)-3-hydroxy-4-phenyl-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]-, methyl ester (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C22 H31 N O4 S  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.  
 Double bond geometry as shown.

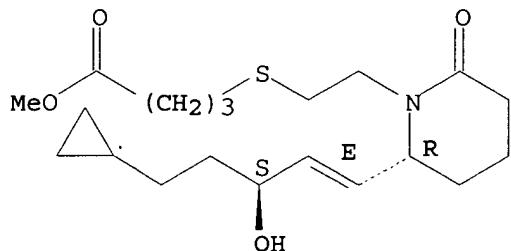


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 724705-99-1 REGISTRY  
 ED Entered STN: 10 Aug 2004  
 CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-5-cyclopropyl-3-hydroxy-1-pentenyl]-6-oxo-1-piperidinyl]ethyl]thio]-, methyl ester (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C20 H33 N O4 S  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.  
 Double bond geometry as shown.

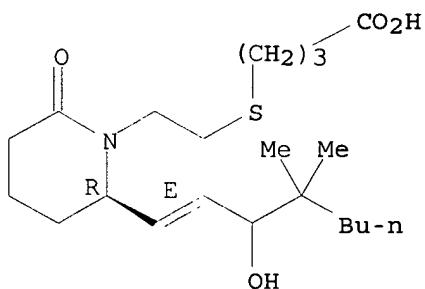


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 724705-80-0 REGISTRY  
ED Entered STN: 10 Aug 2004  
CN Butanoic acid, 4-[[2-[(2R)-2-[(1E)-3-hydroxy-4,4-dimethyl-1-octenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C21 H37 N O4 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.  
Double bond geometry as shown.

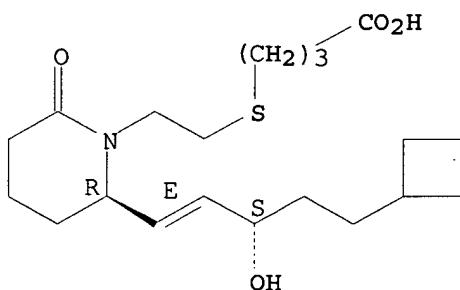


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 724705-78-6 REGISTRY  
ED Entered STN: 10 Aug 2004  
CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-5-cyclobutyl-3-hydroxy-1-pentenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C20 H33 N O4 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.  
Double bond geometry as shown.

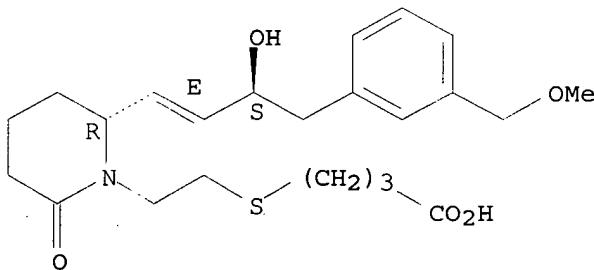


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 724705-74-2 REGISTRY  
ED Entered STN: 10 Aug 2004  
CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-3-hydroxy-4-[3-(methoxymethyl)phenyl]-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C23 H33 N O5 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.  
Double bond geometry as shown.

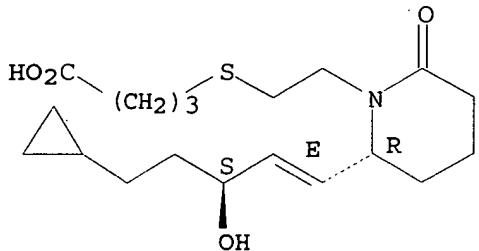


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 724705-66-2 REGISTRY  
ED Entered STN: 10 Aug 2004  
CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-5-cyclopropyl-3-hydroxy-1-pentenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C19 H31 N O4 S  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.  
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus		SINCE FILE	TOTAL
COST IN U.S. DOLLARS		ENTRY	SESSION
FULL ESTIMATED COST		199.10	199.31

FILE 'CAPLUS' ENTERED AT 15:28:56 ON 27 MAR 2007  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 27 Mar 2007 VOL 146 ISS 14  
 FILE LAST UPDATED: 26 Mar 2007 (20070326/ED)

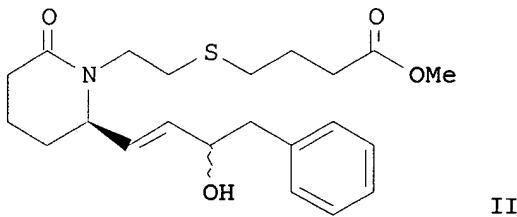
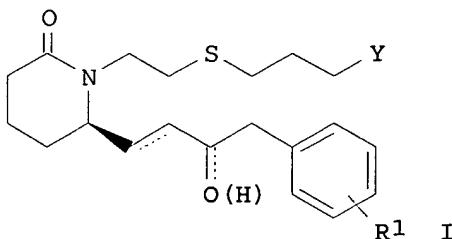
Effective October 17, 2005, revised CAS Information Use Policies apply.  
 They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 13 full  
 L4            3 L3

=> d 14 abs ibib hitstr

L4    ANSWER 1 OF 3    CAPLUS    COPYRIGHT 2007 ACS on STN  
 GI



**AB** 5-Thiopiperidinyl prostaglandin E analogs I [Y = CO<sub>2</sub>H, CONH<sub>2</sub>, CONHMe, CONMe<sub>2</sub>, CONHET, CON(OMe)Me, CON(CH<sub>2</sub>CH<sub>2</sub>OH)<sub>2</sub>, CONH(CH<sub>2</sub>CH<sub>2</sub>OH), CH<sub>2</sub>OH, P(:O)(OH)<sub>2</sub>, CONHSO<sub>2</sub>Me, SO<sub>2</sub>NH<sub>2</sub>, SOI<sub>2</sub>NMe<sub>2</sub>, SO<sub>2</sub>NNHMe, CONH-cyclopropyl, 2H-tetrazol-5-yl; R = C<sub>1</sub>-4-alkyl, C<sub>1</sub>-4-alkoxy, halogen, CO<sub>2</sub>H, OH, CHO, COMe, COCF<sub>3</sub>, NO<sub>2</sub>, CN, CF<sub>3</sub>; dashed line = optional double bond] or a pharmaceutically acceptable salt or a prodrug thereof is disclosed herein. Thus, prostaglandin E thiopiperidinyl analog II was prepared from di-Et (R)-2-aminohexanedioate via N-alkylation with Cl(CH<sub>2</sub>)<sub>2</sub>S(CH<sub>2</sub>)<sub>3</sub>CO<sub>2</sub>Me, intramol. cyclization/amidation, regioselective reduction with LiBH<sub>4</sub>, oxidation and Horner-Emmons reaction with PhCH<sub>2</sub>COCH<sub>2</sub>P(:O)(OMe)<sub>2</sub> and chemoselective reduction with NaBH<sub>4</sub>. A compound II having an ω chain as shown or a derivative thereof, or a pharmaceutically acceptable salt or a prodrug thereof, is disclosed. Methods of treating certain eye conditions or diseases, and compns. and medicaments related thereto are also contemplated.

ACCESSION NUMBER: 2005:1329640 CAPLUS

DOCUMENT NUMBER: 144:69658

TITLE: Methods of preparing 5-thiopiperidinyl prostaglandin E analogs and of treating certain eye conditions or diseases

INVENTOR(S): Old, David W.; Dinh, Danny T.

PATENT ASSIGNEE(S): Allergan, Inc., USA

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005121086	A2	20051222	WO 2005-US17167	20050516
WO 2005121086	A3	20060427		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,			

EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,  
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,  
MR, NE, SN, TD, TG

AU 2005252171 A1 20051222 AU 2005-252171 20050516  
CA 2569464 A1 20051222 CA 2005-2569464 20050516  
EP 1761495 A2 20070314 EP 2005-749871 20050516

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,  
IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR

US 2006281713 A1 20061214 US 2006-564829 20060113

PRIORITY APPLN. INFO.: US 2004-577361P P 20040604  
WO 2005-US17167 W 20050516

OTHER SOURCE(S): CASREACT 144:69658; MARPAT 144:69658

IT 871578-35-7P

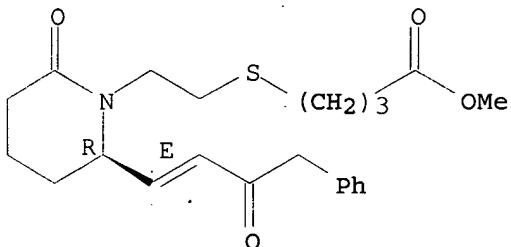
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and borohydride reduction of; preparation of 5-thiopiperidinyl  
prostaglandin E analogs and of treating eye conditions)

RN 871578-35-7 CAPLUS

CN Butanoic acid, 4-[[2-[(6R)-2-oxo-6-[(1E)-3-oxo-4-phenyl-1-butenyl]-1-  
piperidinyl]ethyl]thio]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 871578-25-5P

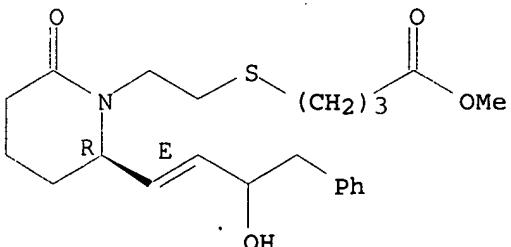
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);  
USES (Uses)  
(preparation and enzymic hydrolysis of; preparation of 5-thiopiperidinyl  
prostaglandin E analogs and of treating eye conditions)

RN 871578-25-5 CAPLUS

CN Butanoic acid, 4-[[2-[(2R)-2-[(1E)-3-hydroxy-4-phenyl-1-butenyl]-6-oxo-1-  
piperidinyl]ethyl]thio]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

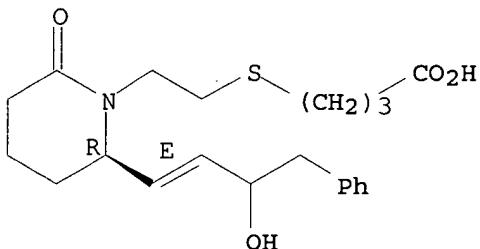


IT 871578-26-6P

RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)  
(preparation of 5-thiopiperidinyl prostaglandin E analogs and of treating  
eye conditions)

RN 871578-26-6 CAPLUS  
CN Butanoic acid, 4-[[2-[(2R)-2-[(1E)-3-hydroxy-4-phenyl-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

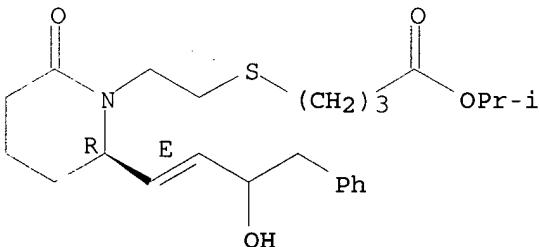
Absolute stereochemistry.  
Double bond geometry as shown.



IT 871578-27-7P 871578-28-8P 871578-29-9P  
871578-30-2P  
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of 5-thiopiperidinyl prostaglandin E analogs and of treating eye conditions)

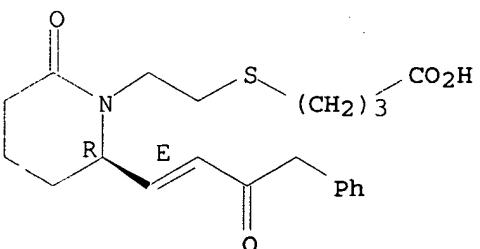
RN 871578-27-7 CAPLUS  
CN Butanoic acid, 4-[[2-[(2R)-2-[(1E)-3-hydroxy-4-phenyl-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



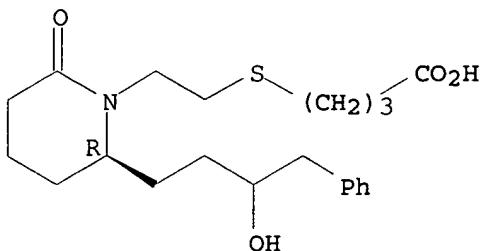
RN 871578-28-8 CAPLUS  
CN Butanoic acid, 4-[[2-[(6R)-2-oxo-6-[(1E)-3-oxo-4-phenyl-1-butenyl]-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RN 871578-29-9 CAPLUS  
CN Butanoic acid, 4-[[2-[(2R)-2-(3-hydroxy-4-phenylbutyl)-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

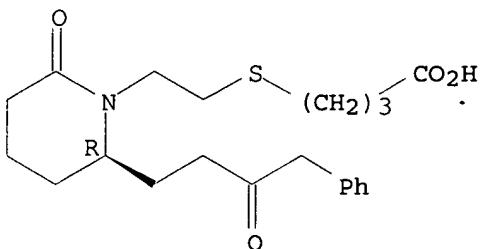
Absolute stereochemistry.



RN 871578-30-2 CAPLUS

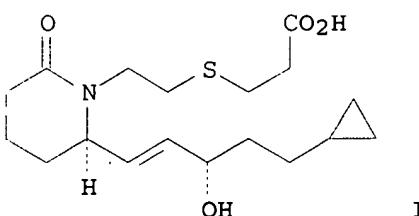
CN Butanoic acid, 4-[(2-[(6R)-2-oxo-6-(3-oxo-4-phenylbutyl)-1-piperidinyl]ethyl)thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d 14 2-3 abs ibib hitstr

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
GI



AB 2-Piperidones, e.g., I, were prepared bearing heptanoic acid or a thioether heptanoic acid at the 1-position as well as appropriately substituted at the 6-position to mimic the structure of prostaglandins. The stereochemical purity at the 6-position was determined to be ≥95% ee for an advanced synthetic intermediate. The 2-piperidones were identified as potent agonists at the EP4 prostanoid receptor. They displayed a high affinity ( $K_i$  5–130 nM) at EP4 and subtype selectivity.

ACCESSION NUMBER: 2005:378879 CAPLUS

DOCUMENT NUMBER: 143:59790

TITLE: Lactams as prostanoid receptor ligands. Part 4:

2-Piperidones as selective EP4 receptor agonists

AUTHOR(S): Elworthy, Todd R.; Brill, Emma R.; Caires, Christopher C.; Kim, Woongki; Lach, Leang K.; Tracy, Jahari Laurant; Chiou, San-San

CORPORATE SOURCE: Roche Palo Alto, Department of Medicinal Chemistry,  
Palo Alto, CA, 94304-1397, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),

15(10), 2523-2526  
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:59790

IT 724705-66-2P 724705-74-2P 724705-78-6P

724705-80-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL  
(Biological study); PREP (Preparation)

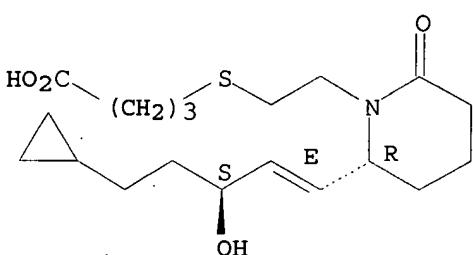
(stereoselective preparation and EP4 receptor binding affinity of  
piperidones starting from amino adipic acid using resolution as the key  
step)

RN 724705-66-2 CAPPLUS

CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-5-cyclopropyl-3-hydroxy-1-pentenyl]-  
6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

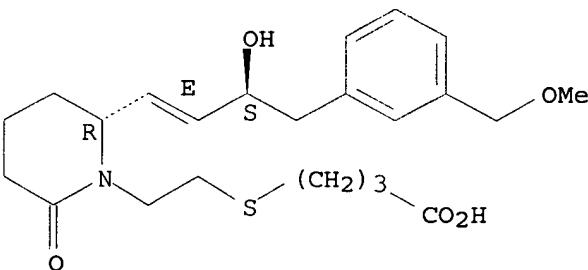


RN 724705-74-2 CAPPLUS

CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-3-hydroxy-4-[3-  
(methoxymethyl)phenyl]-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

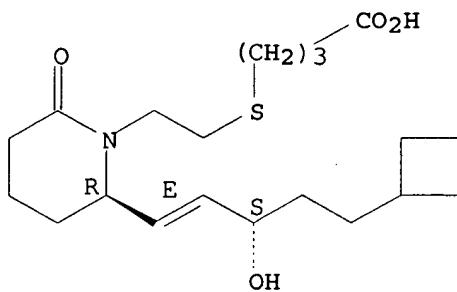


RN 724705-78-6 CAPPLUS

CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-5-cyclobutyl-3-hydroxy-1-pentenyl]-6-  
oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

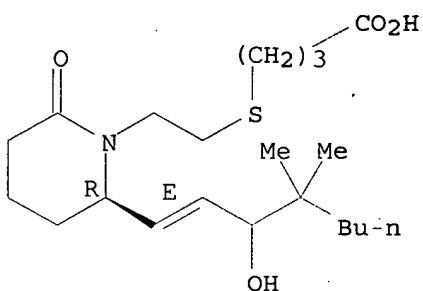


RN 724705-80-0 CAPLUS

CN Butanoic acid, 4-[[2-[(2R)-2-[(1E)-3-hydroxy-4,4-dimethyl-1-octenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

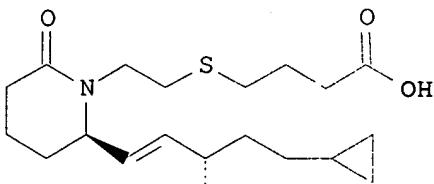
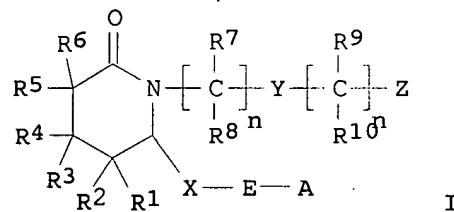
Absolute stereochemistry.

Double bond geometry as shown.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER, 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
GI



II

AB 2-Piperidone derivs. I ( $n = 0-4$ ; A = alkyl, aryl, heteroaryl, arylalkyl, arylcycloalkyl, cycloalkylalkyl, aryloxyalkyl; E = CHO<sub>H</sub>, or C(O); Y = CH<sub>2</sub>, CH:CH, arylene, heteroarylene, O, S(O)<sub>p</sub> ( $p = 0-2$ ); NR<sub>a</sub> (Ra = H, alkyl); Z = CH<sub>2</sub>OH, CHO, tetrazole-5-yl, COOR<sub>b</sub> (Rb = H, alkyl); R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, R<sub>4</sub>, R<sub>5</sub>,

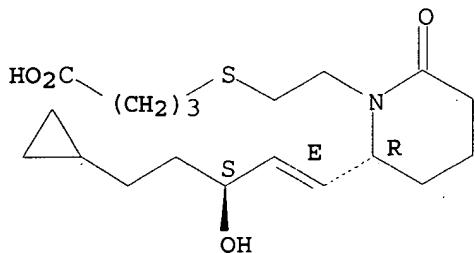
R6, R7, R8, R9, R10 = H, alkyl) and pharmaceutically acceptable salts, solvates, prodrugs, single isomers or racemic or non-racemic mixture of isomers thereof were prepared as selective prostaglandin EP4 agonists for the treatment of associated diseases. Thus, 6R-(1-ethoxy-ethoxymethyl)piperidin-2-one was treated with NaH, and 2-bromoethanol triisopropylsilyl ether, followed by pyridinium p-toluene sulfonic acid to give the alc. The alc. was oxidized to the aldehyde using Swern conditions, and treatment of the aldehyde with (4-cyclopropyl-2-oxobutyl)phosphonic acid di-Me ester gave the alkene. Reduction of the ketone using (R)-2-methyl-CBS-oxazaborolidine followed by deprotection of the silylether gave the primary alc. Treatment of the alc. with γ-thiobutyrolactone gave the Me ester which was treated with NaOH to give the desired II. The invention also provides methods for preparing, compns. comprising, and methods for using compds. of formula I.

ACCESSION NUMBER: 2004:589253 CAPLUS  
 DOCUMENT NUMBER: 141:123513  
 TITLE: 2-piperidone derivatives as prostaglandin agonists  
 INVENTOR(S): Elworthy, Todd Richard  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 26 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004142969	A1	20040722	US 2004-754117	20040108
AU 2004203905	A1	20040729	AU 2004-203905	20040102
CA 2511255	A1	20040729	CA 2004-2511255	20040102
WO 2004063158	A1	20040729	WO 2004-EP8	20040102
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ			
EP 1585729	A1	20051019	EP 2004-700041	20040102
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2004006717	A	20051220	BR 2004-6717	20040102
CN 1735597	A	20060215	CN 2004-80002071	20040102
JP 2006515015	T	20060518	JP 2005-518636	20040102
PRIORITY APPLN. INFO.:			US 2003-439152P	P 20030110
			WO 2004-EP8	W 20040102

OTHER SOURCE(S): MARPAT 141:123513  
 IT 724705-66-2P 724705-74-2P 724705-78-6P  
 724705-80-0P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of 2-piperidone derivs. as selective prostaglandin EP4 agonists for the treatment of associated diseases)  
 RN 724705-66-2 CAPLUS  
 CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-5-cyclopropyl-3-hydroxy-1-pentenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.

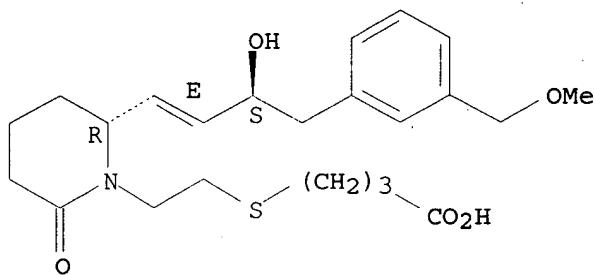


RN 724705-74-2 CAPLUS

CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-3-hydroxy-4-[3-(methoxymethyl)phenyl]-1-butenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

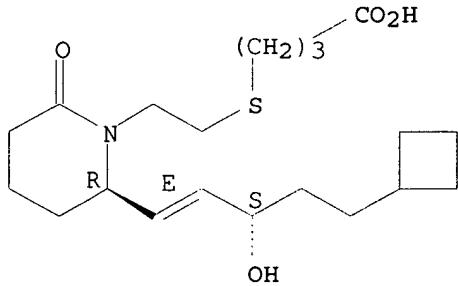


RN 724705-78-6 CAPLUS

CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-5-cyclobutyl-3-hydroxy-1-pentenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

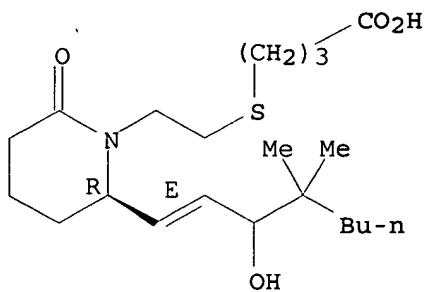


RN 724705-80-0 CAPLUS

CN Butanoic acid, 4-[[2-[(2R)-2-[(1E)-3-hydroxy-4,4-dimethyl-1-octenyl]-6-oxo-1-piperidinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 724705-99-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

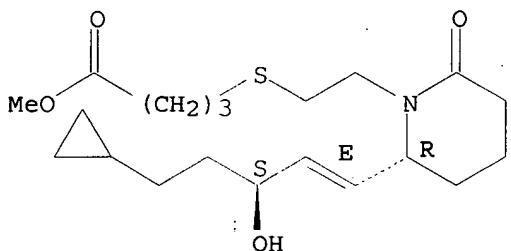
(preparation of 2-piperidone derivs. as selective prostaglandin EP4 agonists for the treatment of associated diseases)

RN 724705-99-1 CAPLUS

CN Butanoic acid, 4-[[2-[(2R)-2-[(1E,3S)-5-cyclopropyl-3-hydroxy-1-pentenyl]-6-oxo-1-piperidinyl]ethyl]thio]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
---------------------	------------------

FULL ESTIMATED COST

19.57 218.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
---------------------	------------------

CA SUBSCRIBER PRICE

-2.34 -2.34

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 15:33:46 ON 27 MAR 2007